

DESIGN, SYNTHESIS, AND PHYSICOCHEMICAL CHARACTERISTICS OF STABLE NITRONYL-NITROXIDE (NNR) DIRADICALS AND THEIR COMPLEXES WITH Cu^{II} BASED ON FUNCTIONAL DERIVATIVES OF ISOPHTHALALDEHYDE

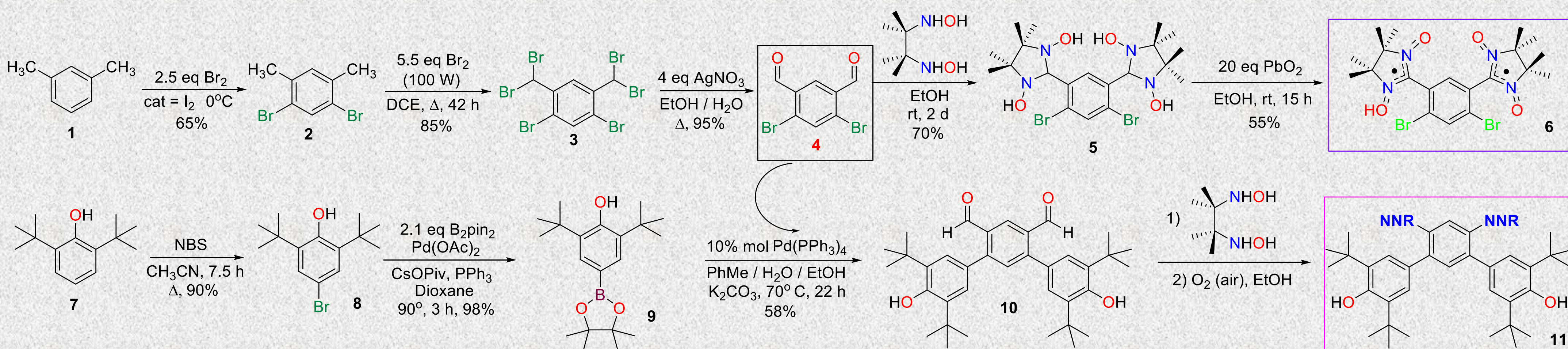
G. W. Khan,^{1,2} T. V. Rybalova,² D. V. Stass,³ D. G. Mazhukin²

¹ NSU, 630090, Russia, Novosibirsk, Pirogova str., 1, ² NIOCH SB RAS, Russia, Novosibirsk

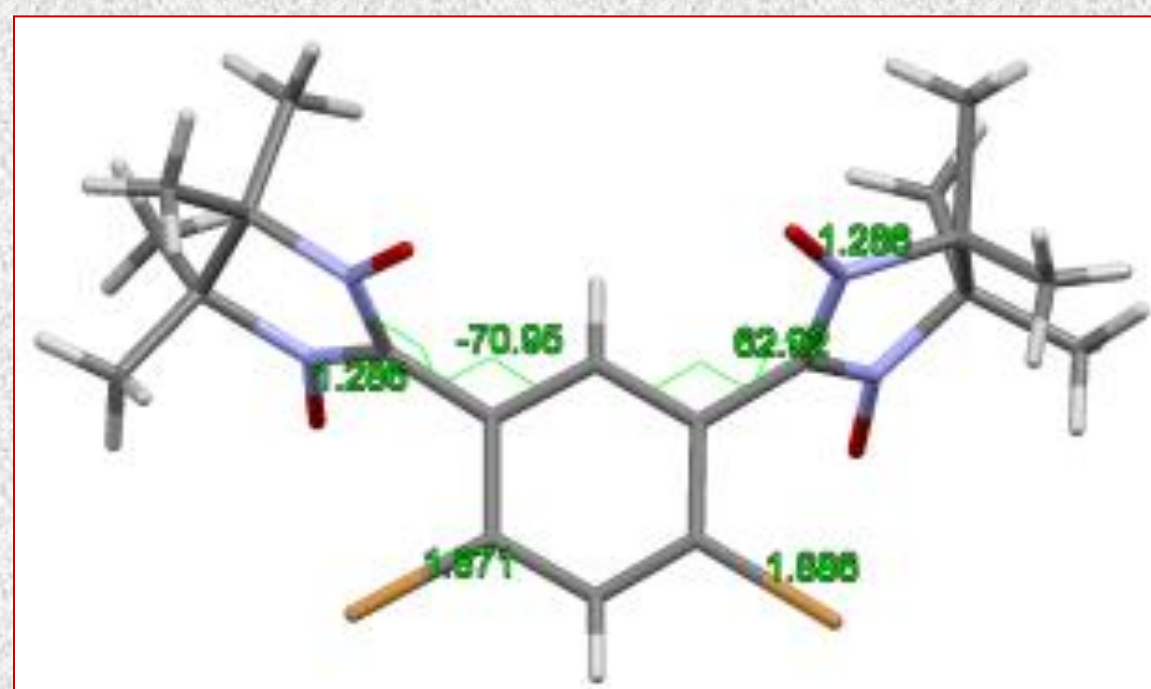
This report discusses methods for obtaining promising synthetic blocks for the synthesis of functionally substituted nitronyl nitroxyl diradicals and their complexes with Cu(hfac)₂ based on *m*-xylene. Using the strategy of Pd-catalyzed cross-coupling reactions of active aryl halides based on 4,6-dibromoisophthalaldehyde, an approach to obtaining a new type of polyhetero-radicals is proposed. In this presentation and poster, various synthetic approaches to previously unknown types of functionally substituted (X, Y = Br, NO₂, COOR, OH) diradicals with *meta*-positioning of the NNR fragments have been discussed.

Part I Synthesis of NNR Diradicals with a two equal functional groups in a benzene linker

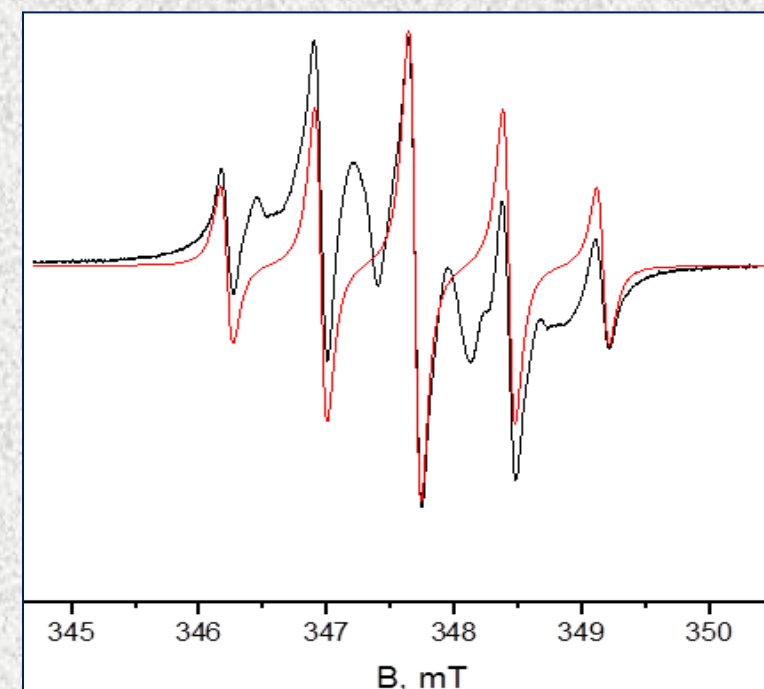
Preparation of diradicals based on 4,6-dibromoisophthalaldehyde



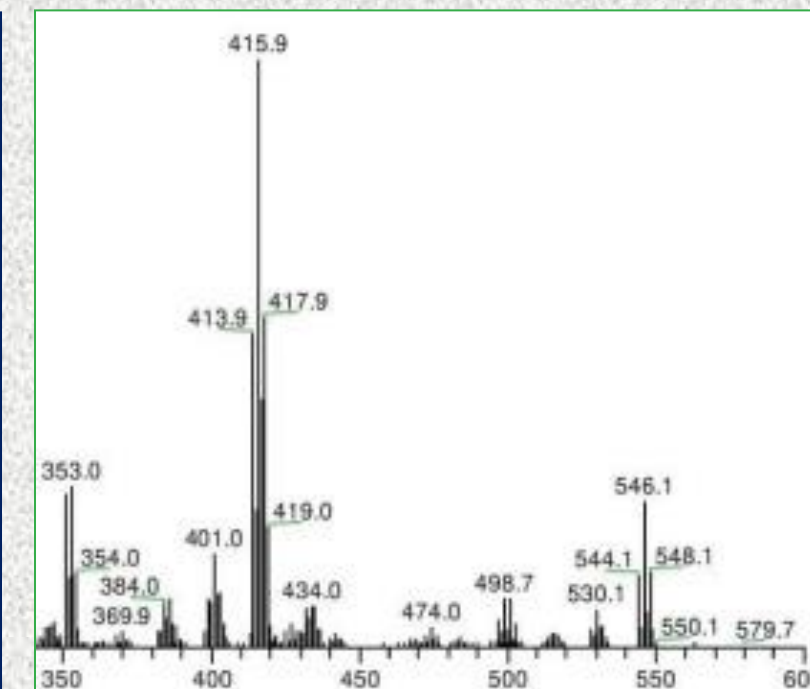
Grown crystals of diradical 6



Resolved X-Ray Structure and EPR-spectrum of Diradical 6

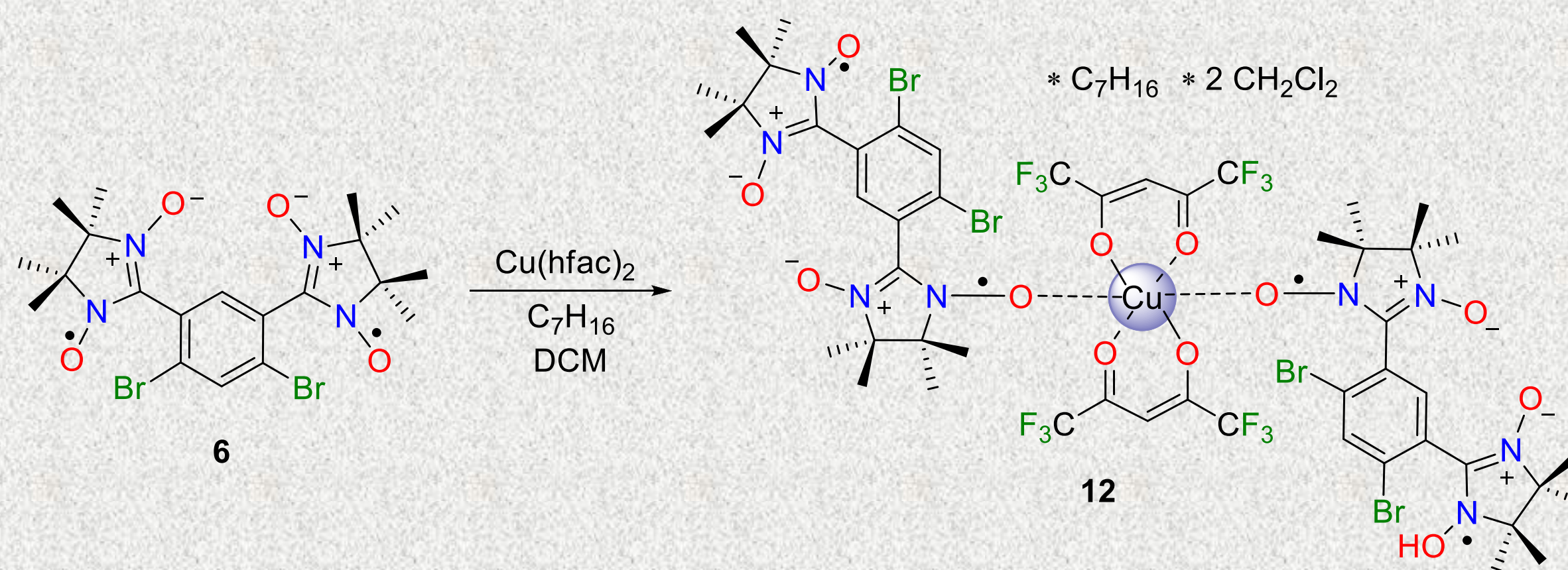


Mass spectrum of Diradical with M-ion at 546



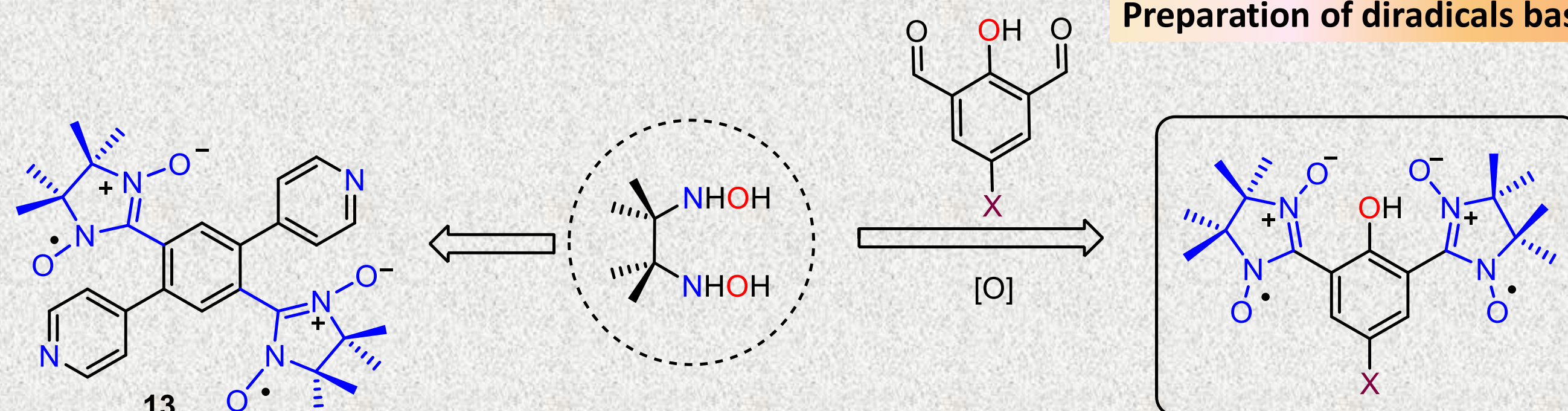
Di-NNR 6 In solution

Synthesis of Cu(II) complex with a diradical 6:

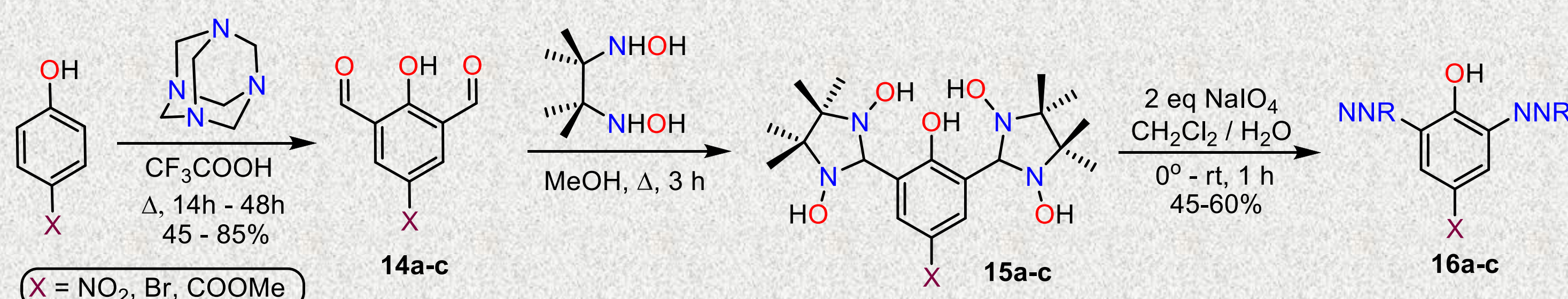


Part II Synthesis of NNR Diradicals with a two different functional groups in a benzene nucleus

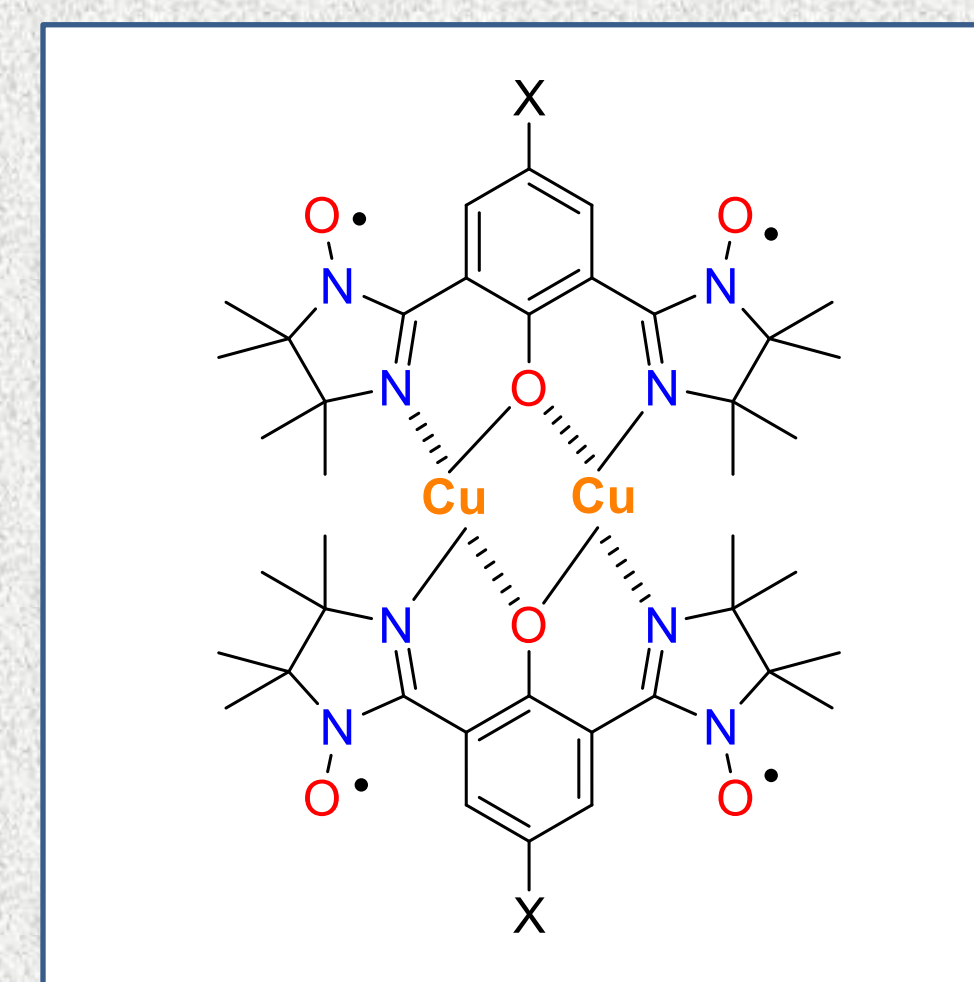
Preparation of diradicals based on p-substituted phenols



S. Volosheniuk et al. *Nat. Commun.*, 2025, 16, 3279.



Immediate plans: to synthesize binuclear Cu(II) complexes with an iminonitroxide diradicals, derivative of 16



The presence of an active halogen or carboxylic function (X=Br, COOH in the molecule of such type of NNR-diradical, could open the route for the creation of multi-spin polynuclear 2D ensembles